



more power to you

Creating Energy Solutions for the Green Age





Dear friends,

In all of American history, the need for our country to develop and embrace the use of new sources of energy has never been as great as it is today. The multiple challenges our country faces — from ensuring our national security to fending off the threat of additional climate change to shoring up a flagging economy — could all be addressed by finding a suite of new, cost-effective and green energy sources.

This issue of *Argonne Now* showcases the work that Argonne's scientists and engineers are doing to create a vibrant energy future for our country. Because there is likely no "silver bullet" that will adequately satisfy all of our energy needs, Argonne's world-class researchers are investigating many different sources of energy — including nuclear, solar and biofuels — as well as ways to store, use and transmit energy more safely, cleanly and efficiently.

As I begin my tenure as Argonne's newest director, I want to reaffirm the laboratory's commitment to creating the groundbreaking technologies and innovations that will secure our country's energy future. This commitment requires reciprocity: in order for us to achieve a sustainable energy future, America must continue to invest in both the basic and applied scientific work that has already produced so many valuable discoveries and inventions.

I would like to take this opportunity to again thank the Department of Energy and all of our many sponsors for providing the means and resources that allow us to carry out this vital research.

Thank you,

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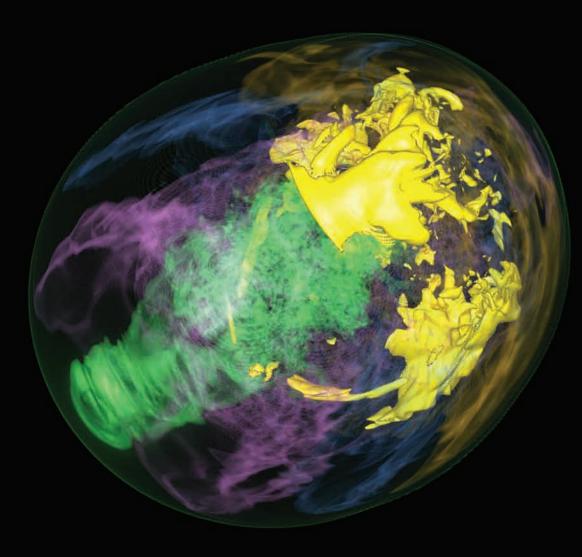
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did you know...

Argonne's "omnivorous engine" consumes many fuels.

news / from Argonne

Argonne scientists are working on more efficient techniques to allow computer visualizations of extremely complex phenomena, like this rendering of a supernova. Generated by Argonne and the University of California at Davis, this image shows the angular momentum at one time step of a simulation of a corecollapse supernova. The data were provided by North Carolina State University and Oak Ridge National Laboratory.



More than just a pretty picture

These days, Argonne researchers generate trillions of separate data points as they research everything from supernovas to protein structures.

In order to make sense of their findings, Argonne's scientists need to be able to graphically interpret their labyrinthine mathematical results. Because even today's most powerful computers are heavily taxed by the process of turning huge quantities of data into understandable images, Argonne's computer scientists are exploring a technique, called software-based

parallel volume rendering, that would speed up visualization.

Volume rendering is a method that can be used to make sense of the vast number of tiny points of data collected from an X-ray, MRI or a researcher's simulation. In order to more efficiently translate the pure data into detailed images, the computer must first divide the data among its many processing cores so that they can all work at once, a technique known as parallel computing.

Usually, the supercomputer's work stops once the data have been gathered, and the data are then sent to a set of graphics processors (GPUs), which create the final visualizations.

Argonne researchers wanted to know if they could improve performance by skipping the transfer to the GPUs and instead create the visualizations on the supercomputer. They tested the technique on a set of astrophysics data and found that they could indeed increase the efficiency of the operation.

Protein puzzlers solve thousandth structure

For nearly a decade, researchers at the Midwest Center for Structural Genomics (MCSG), an international consortium based at Argonne, have been patiently cracking the genetic code of important proteins. Using X-ray crystallography performed at the laboratory's Advanced Photon Source (APS), the Western Hemisphere's most powerful source of X-rays for research, scientists sketch an image of a protein's atomic structure — laying the groundwork for new medical breakthroughs and treatments discovered by scientists all around the world.

On July 17, the MCSG deposited their 1,000th protein

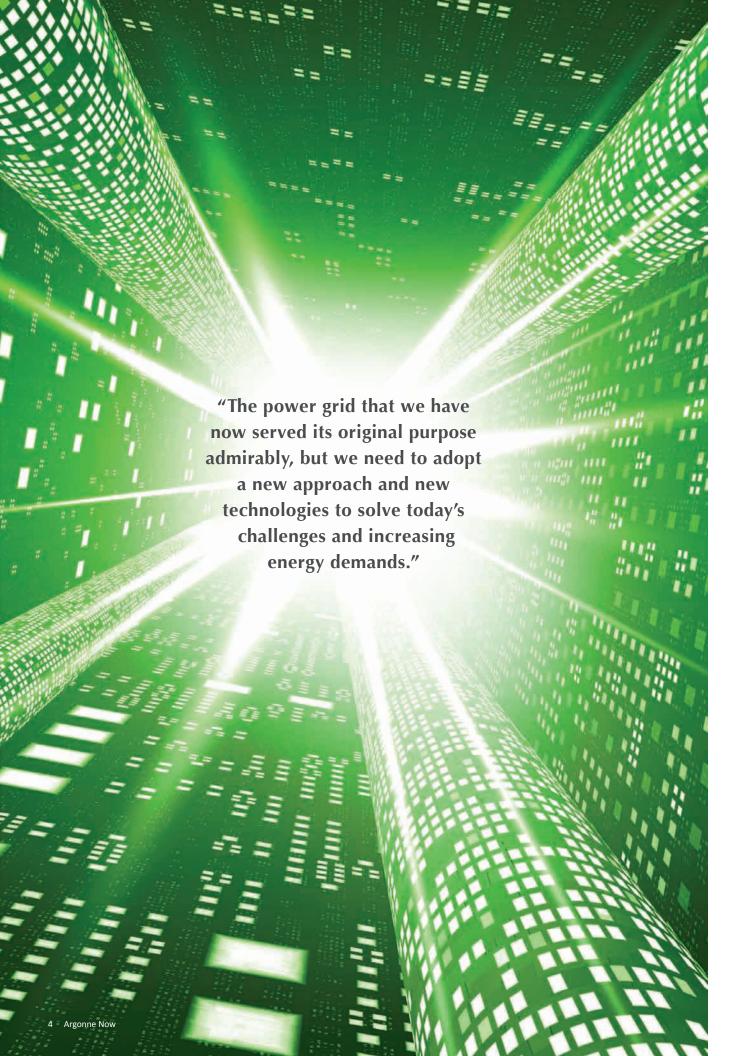
structure into the Protein Data Bank — a collection of known protein structures discovered by scientists all over the world. The MCSG has contributed more structures to the Protein Data Bank than any other institution in the world. In addition, many other institutions, organizations and corporations come to the APS to do protein research. In total, researchers at the APS have contributed over 7,000 structures to the Protein Data Bank.

Founded in 2000, the MCSG works to discover how microbes interact with humans and the environment. It has identified potential new drug targets for anthrax bacteria and shed light on other pathogenic bacteria, including meningitis, salmonella, cholera and staph. After the H1N1 avian flu virus was identified in 2003, the MCSG raced to characterize one of its key proteins, a structure they nicknamed the "dragon" protein for its resemblance to a dragon's head.

"These protein studies provide important clues to the mysteries of human and environmental health by imaging the molecules that control and regulate them," said MCSG director Andrzej Joachimiak. "By visualizing the proteins, we are able to puzzle out the atomic details of how the biomolecule performs its task." (A)



Argonne's Midwest Center for Structural Genomics recently deposited their 1,000th protein structure more than any other organization — into the Protein Data Bank



networks / at Argonne

Knowledge is power

America's power grid system today faces the same kinds of challenges that the country's communication system did in the 20th century. Just as e-mail and telecommunications fundamentally changed how we interact, new technologies for creating, storing and using energy require scientists to find more efficient ways to transmit and distribute it.

In the 127 years since Thomas Edison opened the first commercial power plant, America's electric infrastructure has evolved in ways its designers never anticipated. "Our demand for energy has changed much in the past 50 years, but the ways in which we supply and distribute it really have not," said Mark Petri, Argonne's technology development director. "The power grid that we have now served its original purpose admirably, but we need to adopt a new approach and new technologies to solve today's challenges and increasing energy demands."

Argonne scientists have begun to use the laboratory's computer modeling capabilities to build more comprehensive simulations of electricity generation, distribution and consumption, but they face several challenges. First, although the benefits of new and clean power sources like wind and solar energy are easy to understand, their intermittent nature makes it hard to route power where and when it is needed because certain plants may not be producing electricity at a given moment.

Another challenge lies in the country's transportation system, which has relied on fossil fuels for more than a century. The threat of global climate change has prompted scientists to search for ways to replace fossil fuels with electricity. Plug-in electric vehicles represent a paradigm shift to zero-emission transportation, but millions of such vehicles would

increase electrical demand beyond the capacity of today's power grid. At the same time, these vehicles hold the potential to feed electricity back into the grid during periods of peak demand. Argonne research seeks to efficiently incorporate and evaluate this new way of sharing power.

Finally, effective modeling must integrate the vulnerabilities of the nation's electrical grid, which increase as the grid grows and evolves. The grid makes an attractive target for terrorists or other malefactors who might seek to throw the country's infrastructure into chaos; moreover, a larger, more complex grid system could complicate our ability to anticipate and respond to natural disruptions such as severe weather. The creation of an ideal national power network — one that is simultaneously more efficient and more secure — requires significant innovation in the way we transmit electricity and monitor its use.

Fortunately, Argonne employs a cadre of scientists and engineers who devote their extensive expertise to creating a smarter grid. "By including industrial partners in our effort to remake the grid," Petri said, "we could actually achieve the cost savings and environmental benefits that our models predict."

Argonne and its partners have identified the need for new methods to simulate the national power grid by modeling the creation and flow of electric power as well as the grid's connection to other critical infrastructures, such as transportation, gas, water and communications. Through detailed simulations of how electric power is supplied and transferred around the country, researchers can bolster not only the grid's security but also its reliability, efficiency and resiliency.



Putting the New in Nuclear

Ever since the beginning of the nuclear age, the peaceful use of atomic energy has revolved around the development and commercialization of water-cooled thermal nuclear reactors. Although these reactors have long generated a plentiful, carbon-neutral source of energy, they may soon no longer adequately meet America's nuclear energy needs. Argonne's expertise in designing a more resourceful and cleaner type of nuclear reactor has enabled enormous gains in the efficiency and safety of nuclear power. by Jared Sagoff



For much of the second half of the 20th century, policymakers and scientists believed that newly harnessed atomic power held the key to solving America's energy needs for the indefinite future. The allure of new inexpensive, plentiful energy distracted many Americans from the complications of the new power source.

The 100 or so commercial nuclear reactors in operation in the United States produce radioactive spent fuel that is currently stored at each reactor site, but that now requires a long-term solution. Rising concern about the future of waste storage has prompted a call for a new generation of nuclear reactors that could dramatically reduce the number and size of repositories needed to safely store waste.

Fortunately, Argonne scientists have decades of expertise in creating a different type of reactor that could help to solve both this and other problems. Since the 1950s, Argonne's scientists have worked to develop fast reactors, which allow the recycling of many of the toxic isotopes that compose nuclear waste.

Fast reactors treat spent reactor fuel not as waste but as a rich source of recycled energy. This new kind of reactor system uses a fuel cycle that is better suited to recycling than that of today's light-water reactors.

"The characteristics of the current generation of light-water reactors eventually make the fuel unsuitable for recycling because of its long-term radiological toxicity after it's discharged from the reactor," said Robert Hill, who manages Argonne's Nuclear Systems Analysis department.

"The current fuel cycle is incredibly wasteful," added Hussein Khalil, director of Argonne's Nuclear Engineering Division. "In the earliest days of nuclear power, Enrico Fermi recognized that the conventional uranium fuel cycle was extremely inefficient."

Today, Argonne leads the development of innovative technologies that promise to reduce the cost

of fast reactors and increase their reliability. These technologies include high-performance fuels and materials; compact, low-cost components for the heat transport system; advanced power conversion and refueling systems; and improved capabilities for in-service inspection and repair. Argonne researchers are also advancing a new science- and simulation-based approach for predicting the operating behavior of fast reactors and assuring their safety.

Because they permit the reprocessing of spent nuclear fuel, fast reactors can operate through what is known as the "closed fuel cycle," which dramatically increases the efficiency of uranium use and minimizes the discharge of plutonium and minor actinides as waste. According to Hill, a fast reactor on a closed fuel cycle could — at least theoretically — use 90 percent of the energy available in uranium.

Since fast reactors allow much of the uranium, plutonium and minor actinides to be fully recycled, their final waste products contain little of the extremely long-lived radioactive isotopes. "For every hundred or so repositories you'd need to house the waste from light-water reactors," Khalil said, "you'd only need one for fast reactors that recycled spent fuel to produce the same amount of energy."

The vast majority of commercial nuclear plants use water-cooled reactors that derive their energy from uranium-235, a fissile isotope that splits readily in the reactor core, releasing a great deal of nuclear energy. When a neutron traveling at a sufficient speed collides with uranium-235, the atom splits into two "fission products"— for example, isotopes of krypton and barium — releasing energy and more free neutrons to perpetuate the chain reaction.

However, the fuel used in these reactors is not composed entirely of uranium-235. Roughly 95 percent of the uranium in the fuel is uranium-238 — a non-fissile form of the element. When a low-

energy neutron in a light-water reactor hits uranium-238, it almost always either bounces right off or gets captured by the atom, transforming it into plutonium-239. Like uranium-235, plutonium-239 is highly fissile and thus can also generate tremendous amounts of atomic energy through fission.

As the chain reaction proceeds, a fraction of the neutrons that collide with plutonium-239 are themselves captured instead of causing fission, resulting in the creation of isotopes known as "higher actinides," which are radioactive and long-lived.

To prevent accidental exposure to the long-lived higher actinides and fission products, the spent fuel produced by today's generation of light-water reactors must be isolated from the biosphere in remote areas that will remain geologically stable for tens or even hundreds of millennia. Just a few places in the country provide suitable locations for this kind of storage, and future demand for nuclear energy would only further complicate the selection of storage sites.

Instead of using water, fast reactors employ a coolant — typically liquid sodium — that does not "moderate," or slow down, neutrons. The resulting "fast" neutrons are not as easily captured, and instead are more likely to split most actinides.

In addition to discharging less hazardous material than conventional reactors, fast reactors use uranium much more efficiently. In a light-water reactor, the initial fuel must be enriched to include a higher fraction of the fissile U-235; the large amount of U-238 discarded in the enrichment process is basically wasted.

Moreover, only about five percent of the enriched fuel can be consumed in the reactor if its physical integrity is to remain assured. "It's not like a car where you can take your tank all the way to empty," Khalil explained. "As you burn the uranium, the chain reaction eventually fizzles out and the fuel properties deteriorate. By the time you've gone through about

five percent of your fuel, you just have to take the rest out and replace it with fresh fuel. All in all, you're using only about one percent of the uranium you took from the ground."

Conversely, with fast reactors, fewer neutrons are captured by the actinides and fission products, resulting in a more favorable neutron balance. The extra neutrons convert U-238 into fissile material, allowing it to be consumed almost entirely by fission and repeated fuel recycling.

Energy companies have not yet scaled up and fully commercialized fast reactor technology, not because of any inherent deficiency in fast reactor technology or operation, but because fresh uranium remains plentiful and cheap. "Right now, light-water reactors make more economic sense because the infrastructure for them is already established," Khalil said. "But the day may not be too far off when spent fuel accumulation and uranium scarcity become serious problems requiring other solutions."

The United States currently faces, or may soon face, challenges in how it disposes of nuclear spent fuel and how efficiently it uses uranium. Today's commercial nuclear technologies do not offer viable long-term solutions to either of these challenges. Just as for other energy technologies, innovations in nuclear energy developed at Argonne help guarantee a safe, affordable and environmentally friendly component of our country's energy supply.

"The vision, drive and knowledge of fast reactors and fuel recycling still reside at Argonne," Hill said. "We have taken the lead in making sure that the world recognizes their role in securing America's energy future."





Solving America's energy challenges will require contributions from many different energy technologies, but one form of energy holds special promise because it is both abundant and also virtually pollution-free: solar power.

In one hour, more solar energy falls on the Earth's surface than the whole world uses in a year. "If you thought of powering America as trying to fill a swimming pool," said Argonne materials scientist George Crabtree, "then the energy from the sun's rays would give you enough to fill Lake Michigan."

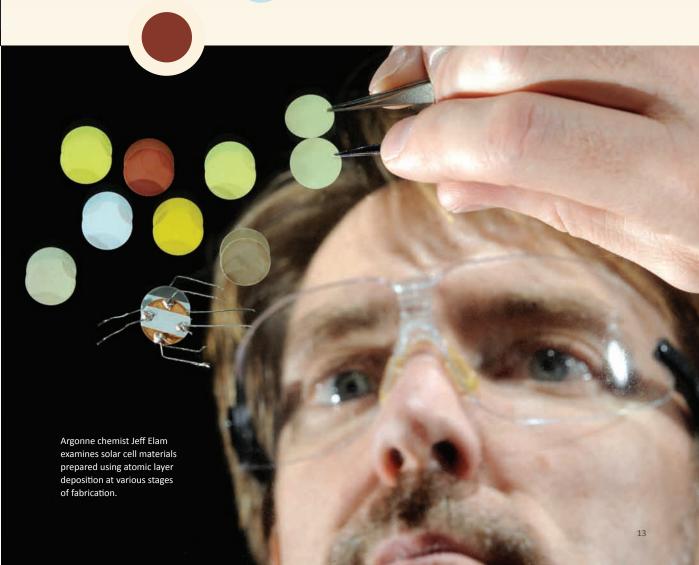
To develop its capabilities in solar energy research, Argonne has brought together expertise from across the laboratory and from partner institutions to form a unified systems approach to solar energy. An additional collaboration between the laboratory and Northwestern University has also taken root as part of the U.S. Department of Energy's Energy Frontier Research Center initiative. The Argonne-Northwestern Solar Energy Research Center (ANSER) brings scientists together to understand and control the chemical processes and materials necessary to obtain cheap, efficient and clean solar energy. Researchers at ANSER

investigate converting solar energy to both electricity and fuel.

Solar panels convert sunlight to electricity through the photovoltaic effect, a process by which a semiconducting material absorbs energy-carrying photons, which are "bundles" of light. Once absorbed by the semiconductor, these photons knock loose electrons, leaving behind a region of positive charge called a "hole." The electron and hole move in opposite directions through a circuit, creating electricity.

The vast majority of the initial research in solar cell technology focused on crystalline silicon, one of the most common and efficient semiconductors for photovoltaics. Even under optimal conditions, however, a perfect single-junction silicon crystal could convert sunlight to electricity at an efficiency of only about 30 percent. The prohibitive cost of systems based on these single-junction crystals — which cost approximately \$10 per watt — prevents them from competing with fossil fuels, which provide power at roughly \$2 a watt when capital costs are taken into account.

"If you thought of powering America as trying to fill a swimming pool, then the energy from the sun's rays would give you enough to fill Lake Michigan."



"Silicon is already almost as efficient as it can be," said Argonne nanoscientist Seth Darling, who is Argonne's solar strategy leader. "The reason we're not putting it on roofs everywhere is that it's just so expensive. Silicon and other current technologies by themselves are never going to be cost-competitive with fossil fuels on a global scale."

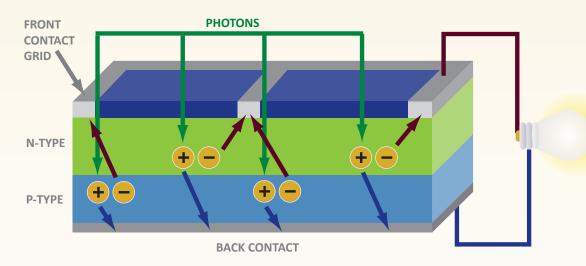
In order to eventually provide clean solar energy at a cost close to that associated with fossil fuels, scientists need either to improve the efficiency of their solar cells or dramatically cut the cost of the materials and processes needed to produce them. As a result, scientists from around the world have begun to investigate a number of materials that could help to promote the photovoltaic effect.

Most of these newer and cheaper substances — which range from photosensitive dyes incorporated in oxide nanomaterials to organic or inorganic thin films — convert sunlight much less efficiently than crystalline silicon-based solar cells. According to Argonne senior materials scientist and Materials Science Division director Michael Pellin, the cost savings associated with the use of these technologies can compensate for their lower efficiencies, but the sheer land area required for enough of these solar cells to completely replace fossil fuels prevents their immediate adoption.

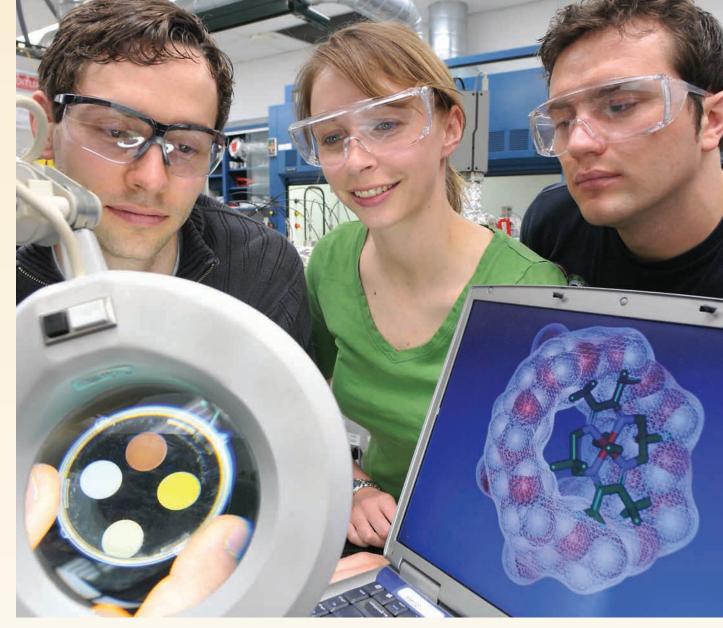
"If you wanted to satisfy all of the country's energy needs with 10-percent-efficient solar cells, you'd need to produce and install panels that would cover an area equal to that of all the federal highways in America," Pellin said. "We've taken on projects of a similar scale before, but it would obviously be extraordinarily difficult."

One of the major complications that dramatically reduces the efficiency of low-cost solar cells involves the short lifespan of the electron-hole pair, also known as an "exciton." In order for the two constituent charges of the bound exciton to successfully separate and produce electricity, the two opposing regions of semiconducting material — one conducts electrons, the other holes — have to be within 10 nanometers of each other. Otherwise, the material will lose the energy it has just absorbed.

Simply stacking two ultrathin layers of semiconductors, however, would create solar cells that would not absorb as many photons. To satisfy the exciton's requirement for closely packed layers of semiconducting material, Argonne materials scientists are perfecting various techniques for controlling the three-dimensional nanoscale structure within low-cost photovoltaic materials.



This illustration of a solar cell shows photons hitting a photoreceptor, creating a bound pair of opposite charges — called an "exciton" — as they enter the semiconductor. At the boundary between the two semiconducting materials, the exciton splits as the charges each get pulled in opposite directions, creating an electric current.



Postdoctoral appointees Ioan Botiz (left), Karen Mulfort and Alex Martinson are exploring the possibility of coupling photovoltaic devices (magnifier) and solar fuel (monitor).

One such approach is called atomic layer deposition, which allows Argonne's nanoscientists to precisely place thin films of conducting oxides and semiconducting materials on the inside of nanoporous membranes. The interspersing of the different semiconductor types enables many more of the excitons to split, improving the material's electrical efficiency.

The utility of solar energy does not begin and end merely with the creation of new photovoltaic materials.

In his work as the solar strategy leader, Darling strives to incorporate the conversion of solar energy with other facets of the energy system. "Photovoltaic cells are just one piece of the solar puzzle," Darling said. "Our strategy is to combine our other areas of expertise — for example, in interface science, grid modeling and energy storage — to create an overarching solar energy program that will ultimately allow sunlight to meet a greater share of our ever-growing energy needs."

Charging
Ahead

The development of lithium-ion batteries for hybrid electric vehicles generated a paradigm shift by creating the potential for the full electrification of the America's transportation network. Although the current generation of plug-in hybrid electric vehicles (PHEVs) cannot travel very far on a single charge, Argonne's transportation engineers have made groundbreaking discoveries that promise to bring the country ever closer to a zero-emissions transportation future.

by Jared Sagoff





Every six months, we're reminded to change the batteries in our household appliances: smoke alarms, flashlights and radios. But what if you had to change the battery in your all-electric car just as often? That's one of the problems that face the generation of lithiumion batteries used in today's all-electric vehicles.

Fortunately, researchers at Argonne, as part of the laboratory's multi-pronged effort to improve energy-storage technology, may have found a way to exponentially increase the calendar and cycle lifetimes of lithium-ion batteries. Electric double-layer capacitors — conventionally known as "ultracapacitors" — have an energy density thousands of times greater than conventional capacitors and a power density hundreds of times greater than lithium-ion batteries.

In an electric vehicle drivetrain, energy density provides sustained speed, while power density facilitates acceleration. "Energy density is what allows you to run a marathon; power density is what enables you to sprint," said Ted Bohn, an automotive engineer in Argonne's Center for Transportation Research.

"Ultracapacitors aren't of much use just by themselves," he added, "but when you couple them with lithium batteries, they dramatically boost the performance of the entire vehicle."

When an electric vehicle merely needs to maintain a particular speed, it requires little of the battery's

power density. However, when the car needs to accelerate from a standstill to a cruising velocity, today's lithium-ion batteries must strain to provide the necessary oomph. "Ultracapacitors," Bohn said, "give an electric vehicle that initial boost it needs to get going."

According to Bohn, commercially available lithium-ion batteries retail for thousands of dollars. A purely electric car that lacked the extra power density supplied by ultracapacitors would permanently burn out its battery within a matter of months. Without ultracapacitors, the cost of replacing such an expensive part during regular maintenance has complicated the development of economically competitive zero-emissions vehicles.

Today's hybrid cars recharge their batteries by transforming kinetic energy from the wheels into potential electrical energy as the driver brakes. Conventional lithium-ion batteries, however, absorb this energy slowly and inefficiently. By contrast, ultracapacitors, because of their immense internal surface area, soak up reclaimed energy like a sponge. "By integrating the entire system," Bohn said, "we can drive down the cost. When we can put these various electronic elements together, we'll transform an \$8,000 battery into a \$4,000 all-electric drivetrain system."

>>> text continued on page 20



Unlike today's petroleum economy, the electrification of the country's transportation network would offer consumers a much broader range of options when purchasing energy.

Smart-charging stations developed by Argonne in conjunction with Swedish researchers would allow electric vehicle drivers to tailor their energy consumption to their own preferences. A radio-frequency identification chip would store information on whether a driver preferred to use fossil, nuclear, solar, water or wind power as well as his or her price sensitivities. Plug-in vehicle technology also represents a two-way street between the car and the grid, because drivers can opt to sell energy back to the grid during periods of high demand when their cars are not in use. Here are a few examples of how drivers with different inclinations could fuel their cars in different ways:



Joanna is a hotshot attorney on travel for business. She stops to refill her plug-in at a charging station right outside of Chicago. Since she's on a corporate account, Joanna cares mostly about the availability of fuel and not its price or whether it is produced by coal, solar or nuclear plants.



Kevin works as the director of an environmental nonprofit. He's keen on practicing what he preaches, and that means fueling his plug-in with carbon-neutral energy, even if he has to pay more for it or wait a little longer for his battery to fully recharge.



Lisa is a college student on a long-distance drive home to visit her family for a week. When she stops into the charging station to refuel, her biggest concern is the price she's paying at the "pump." She can configure her settings so that her car is always fueled with the most inexpensive available energy, regardless of its environmental impact.

A New "Energy Frontier"

Ultracapacitors represent only one tool that Argonne scientists and engineers are using to solve today's pressing challenges in electrical storage. This past April, the U.S. Department of Energy announced that Argonne will host a new Energy Frontier Research Center devoted to energy storage research. This new facility, which will be called the Center for Electrical Energy Storage (CEES), will bring together a team of 17 world-class researchers from Argonne, Northwestern University and the University of Illinois at Urbana-Champaign.

At its core, CEES will draw on Argonne's vast expertise in lithium-ion battery technology. "There is a tremendous amount of innovation that can happen just within lithium-ion technologies," said Mark Peters, deputy associate laboratory director for energy sciences and engineering. Argonne's three-year-old Center for Nanoscale Materials offers a new set of capabilities and resources that scientists and engineers can use to dramatically improve lithium-ion batteries.

However, no matter how far energy storage technology may develop in the laboratory, basic scientists must connect with industrial partners in order for CEES discoveries to make their way into cars on the dealership lot. The American Reinvestment and Recovery Act, passed this spring, allocated more than \$2 billion for domestic battery manufacturing, and Argonne has already started building relationships with other institutions to work toward that goal.

In April, the laboratory reached an agreement with the Commonwealth of Kentucky, the University of

Kentucky and the University of Louisville to create a joint battery manufacturing R&D center that will be located in central Kentucky and at Argonne. "Perhaps the biggest challenge in battery technology today is setting up a significant manufacturing presence in the United States," Peters said. "The batteries that are currently in hybrid vehicles and planned for plug-in hybrid vehicles, like the Chevy Volt, and ultimately electric cars, all come from Asia; we can create a lot of jobs and save a lot of money by doing the same work

As it gradually weans America's transportation infrastructure from its dependence on fossil fuels, advanced storage technology also offers the opportunity for electrical consumers to transfer energy back to the electrical grid during periods of peak demand. The wall outlet for charging a plug-in hybrid could easily form a two-way connection between the consumer and the grid; when the car's battery will not be needed for a certain length of time, the owner could sell the battery's energy back into the grid when power is priciest — say, during the mid-afternoon on a hot summer day — then refill the battery overnight when the price of electricity has fallen.

"Research in new storage technologies and research in grid improvements have, until now, proceeded along two largely separate paths," Peters said. "As we begin to electrify the transportation sector, we're faced with a great opportunity to bring together the benefits that both of these fields of study will produce." 🛆



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smart grid

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did you know...

Argonne mechanical engineer Thomas Wallner makes an adjustment to the laboratory's "omnivorous engine."

...that although today's automobile engines typically run solely on gasoline or, in rare instances, on a blend of gasoline and ethanol, Argonne scientists are developing an "omnivorous engine" (pictured above) that would be able to run on any blend of conventional gasoline, ethanol or butanol, another organic alcohol that scientists are beginning to consider as a potential biofuel. The omnivorous engine comes equipped with a suite of sensors to calibrate the engine to burn available fuel as efficiently as possible.

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